Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.60e-07 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.18e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

Image not found
Dieldrin
Measured: 5.80e-07
Predicted: 3.60e-07

Image not found
Endrin
Measured: 5.80e-07
Predicted: 3.60e-07

Image not found
Heptachlor epoxide
Measured: 5.14e-07
Predicted: 3.52e-07

Image not found
Endrin aldehyde
Measured: 6.30e-08
Predicted: 1.07e-07

Image not found
Heptachlor
Measured: 4.82e-07
Predicted: 3.17e-07

Image not found
Aldrin
Measured: 4.66e-08
Predicted: 9.23e-08